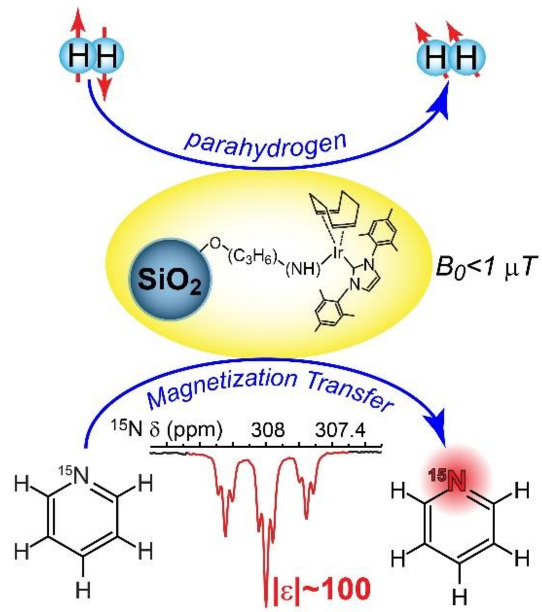
ENHANCING NMR AND MRI WITH HYPERPOLARIZATION (Goodson Lab)

Low detection sensitivity remains an Achilles Heel of many conventional NMR/MRI methods, particularly for dilute substances. However in some circumstances, highly-non-Boltzmann nuclear spin population distributions can be generated to create "hyperpolarized" (HP) species that can be used to improve the NMR detection sensitivity by orders of magnitude.

Development of Novel Catalysts and Approaches for "SABRE" Enhancement of NMR and MRI. In a technique pioneered by the York group called SABRE (Signal Amplification by Reversible Exchange) the pure spin order of parahydrogen (pH_2) may be partially but rapidly transferred to target substrate molecules. Importantly, SABRE needs an organometallic catalyst to work by transiently co-locating pH_2 and the substrate. Our objective is to develop new materials and approaches that will dramatically improve the efficiency and applicability of SABRE. For example, we are working to increase SABRE efficiency for heteronuclei (^{15}N, ^{13}C, etc.) by performing SABRE inside a magnetic shield, where the sub-micro-Tesla magnetic field is small enough to allow efficient transfer of spin order via scalar couplings. We have also been working to create "HET-SABRE" catalysts where SABRE catalytic moieties are immobilized onto various solid supports—including the recent combination of both approaches to enhance ^{15}N NMR signals via "HET-SABRE" using a magnetic shield (see **Figure**). In addition to greatly improving "HET-SABRE" efficiency, we are working to achieve facile separation of hyperpolarized molecules from the catalysts (made possible by their heterogeneous nature) to enable applications and catalyst reuse. Towards those ends, **REU students** will learn how to synthesize homogeneous and heterogeneous SABRE catalysts (including via glove-box methods). The REU students will use many techniques (including NMR, AAS, EM, MS, DLS, etc.) to characterize the catalysts, and NMR to optimize the resulting signal enhancements under different conditions (e.g. concentrations, substrate choice, catalyst and support structures, support surface-to-volume ratio, mixing magnetic field strength, temperature, etc.). Ultimately, our research efforts will provide greater insight into SABRE approaches, while working to dramatically improve their utility for a wide range of NMR/MRI applications, including HP low-field imaging of living organisms.



Bubbling parahydrogen gas into a solution containing a heterogeneous iridium-based catalyst (immobilized on silica supports) can produce greatly enhanced heteronuclear (e.g. ^{15}N) NMR signals when performed inside a magnetic shield prior to transfer to an NMR spectrometer for acquisition.

Fundamentals and Applications of Hyperpolarized Xenon. Another approach of interest to our laboratory involves the creation of hyperpolarized xenon-129 (HPXe) via spin-exchange optical pumping (SEOP). In SEOP, a high-power near-infrared laser is used to polarize the electron spins of an alkali metal vapor (like rubidium or cesium); the high spin polarization may then be transferred to the nuclear spins of noble gases like xenon during gas-phase collisions. The nuclear spin polarization can accumulate over time until it is several orders of magnitude higher than what is obtained at thermal equilibrium (in even the strongest magnets), thereby rendering the gas "hyperpolarized". Projects along these lines include (1) fundamental studies of SEOP processes; (2) technical efforts to improve laser technology, increase the nuclear spin polarization efficiency, and develop xenon "hyperpolarizers"—devices for clinical-scale production of HPXe; and (3) applications of HPXe (including materials and biomedical imaging applications).